Quantum Mechanics

Schrödinger equation

Problem 1.- Write the Schrödinger equation in spherical coordinates for the potential

$$V(r) = -\frac{K}{r^2}$$

Solution: In three dimensions and using spherical coordinates, the Schrödinger equation has the form

$$-\frac{\hbar^2}{2m}\nabla^2\psi(R,\theta,\phi) + V\psi(R,\theta,\phi) = E\psi(R,\theta,\phi)$$

With the potential function given, the equation will have the specific form:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(R,\theta,\phi) - \frac{K}{r^2}\psi(R,\theta,\phi) = E\psi(R,\theta,\phi)$$

To solve the equation, we could start by separating variables and solving the angular part first.

Problem 2.- Write the Schrödinger equation in spherical coordinates for the potential

$$V(r) = \frac{C}{r^6} - \frac{C'}{r^{12}}$$

Solution: The Schrödinger equation in spherical coordinates for the potential given is:

$$-\frac{\hbar^2}{2m}\nabla^2\psi(R,\theta,\phi) + \left(\frac{C}{r^6} - \frac{C'}{r^{12}}\right)\psi(R,\theta,\phi) = E\psi(R,\theta,\phi)$$

Problem 3.- Find the eigen energies of the Hamiltonian:

$$H = E_o\begin{pmatrix} 0 & 3 \\ 3 & 0 \end{pmatrix}$$

Solution: To find the eigen energies, we make the determinant of H-EI zero:

$$\det(H - EI) = \det\begin{pmatrix} -E & 3E_o \\ 3E_o & -E \end{pmatrix} = E^2 - 9E_o{}^2 = 0 \rightarrow E = \pm 3E_o$$

Problem 4.- Find the eigen energies and eigen functions of the Hamiltonian:

$$H = E_o \begin{pmatrix} 0 & 2 & 0 \\ 2 & 0 & 0 \\ 0 & 0 & 5 \end{pmatrix}$$

Solution: To find the eigen energies, we make the determinant of H-EI zero:

$$\det(H - EI) = \det \begin{pmatrix} -E & 2E_o & 0 \\ 2E_o & -E & 0 \\ 0 & 0 & 5E_o - E \end{pmatrix} = 0$$

This translates into an algebraic equation:

$$(5E_o - E)(E^2 - 4E_o{}^2) = 0 \rightarrow E = 5E_o, \pm 2E_o$$

For each eigen energy there will be one eigenvector:

For E = $5E_o$

$$\begin{pmatrix} -5E_o & 2E_o & 0 \\ 2E_o & -5E_o & 0 \\ 0 & 0 & 5E_o - 5E_o \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = 0 \rightarrow \psi_1 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

Notice that the eigenvector is already normalized.

For E = $2E_o$

$$\begin{pmatrix} -2E_o & 2E_o & 0 \\ 2E_o & -2E_o & 0 \\ 0 & 0 & 5E_o - 2E_o \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = 0 \rightarrow \psi_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

The factor $\frac{1}{\sqrt{2}}$ is necessary to normalize the eigenvector.

For E = $-2E_o$

$$\begin{pmatrix} 2E_o & 2E_o & 0 \\ 2E_o & 2E_o & 0 \\ 0 & 0 & 5E_o + 2E_o \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = 0 \rightarrow \psi_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$$

Problem 5.- Find the eigen energies of the Hamiltonian

$$\mathrm{H} = \mathrm{E_o}\begin{pmatrix} 1 & \delta \\ \delta & 2 \end{pmatrix}$$

What happens if $\delta = 0$?

Solution: To find the eigen energies of the Hamiltonian we look for values of E that make the determinant of H-EI equal to zero

$$\det(H - EI) = \det\begin{pmatrix} E_o - E & \delta E_o \\ \delta E_o & 2E_o - E \end{pmatrix} = (E_o - E)(2E_o - E) - \delta^2 E_o{}^2 = 0$$

Solving for E

$$2E_o{}^2 - 3EE_o + E^2 - \delta^2 E_o{}^2 = 0 \rightarrow E^2 - 3EE_o + 2E_o{}^2 - \delta^2 E_o{}^2 = 0$$

$$E = \frac{3E_o \pm \sqrt{9E_o{}^2 - 4(2E_o{}^2 - \delta^2 E_o{}^2)}}{2} = \frac{3E_o \pm \sqrt{E_o{}^2 + 4\delta^2 E_o{}^2}}{2} = \frac{E_o\left(3 \pm \sqrt{1 + 4\delta^2}\right)}{2}$$

If $\delta = 0$ the solutions would be: $E = E_o$ and $E = 2E_o$